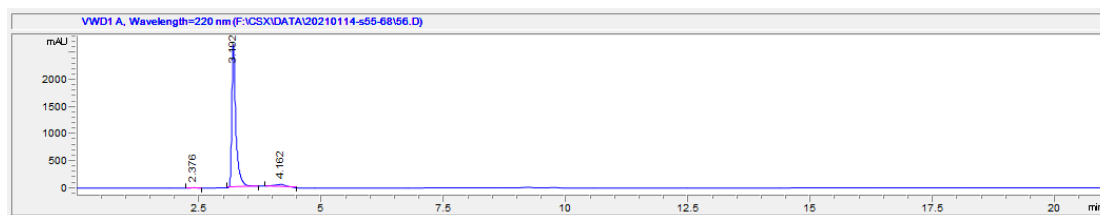
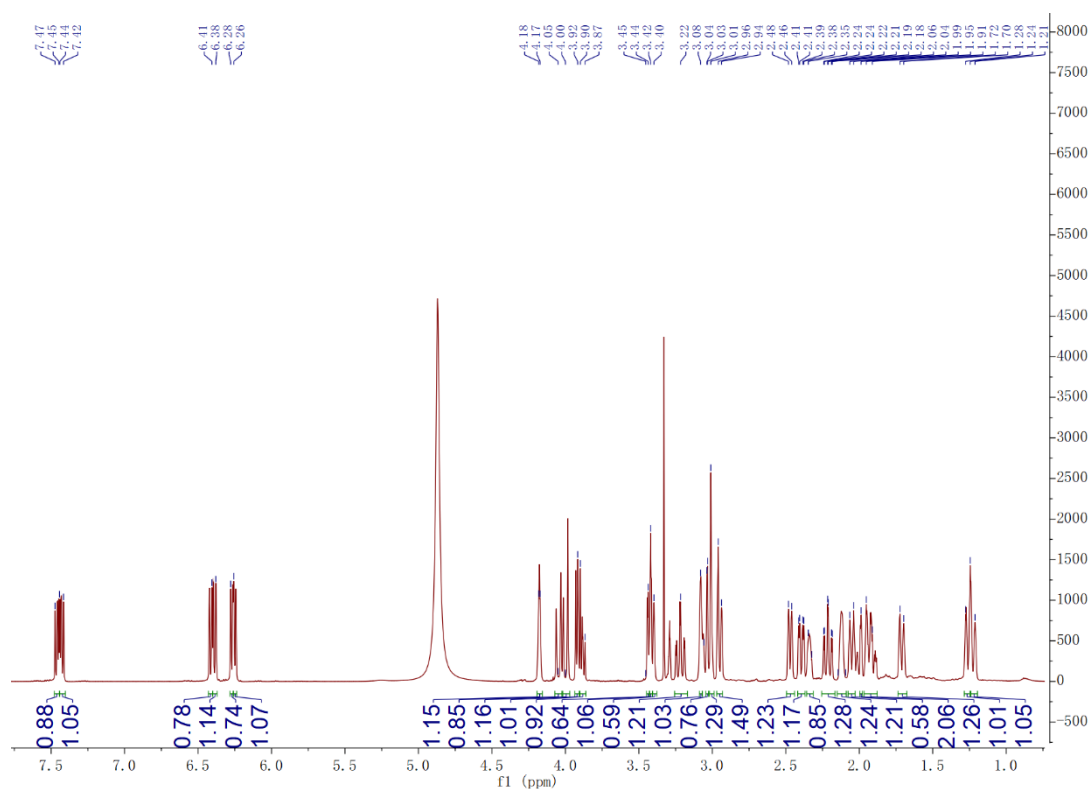


## Supplementary Data

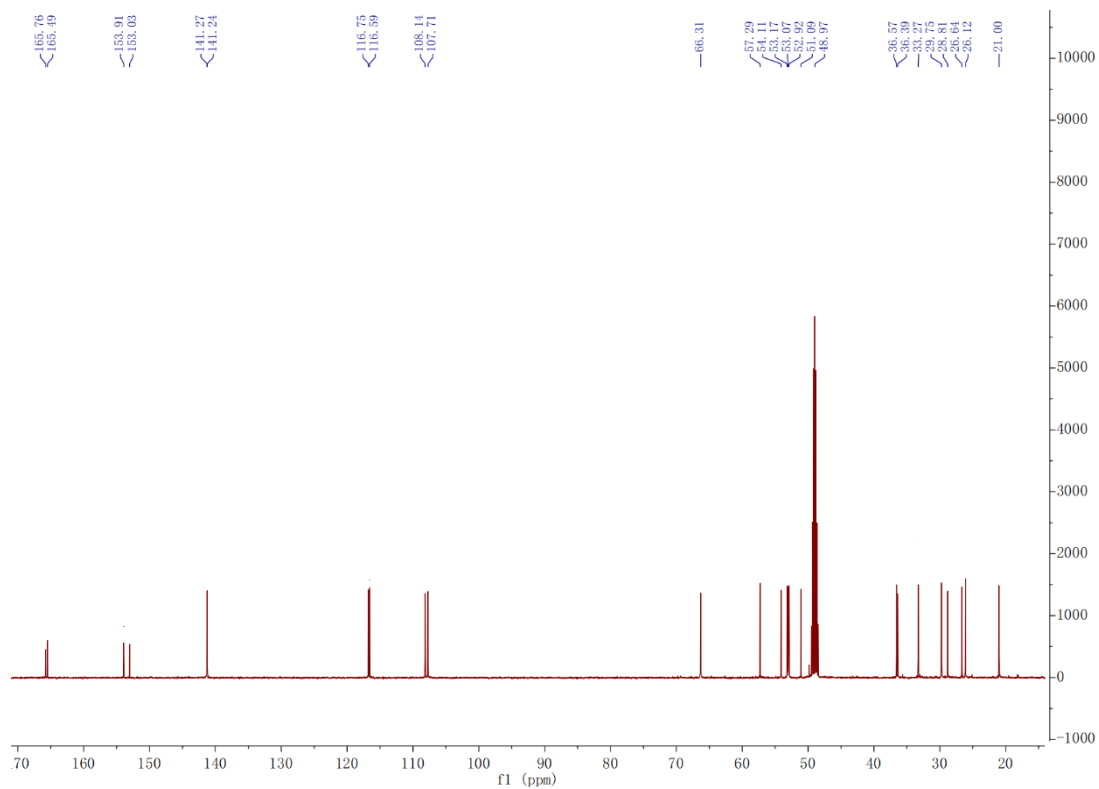


Number	Retention Time	Peak Area% (Area Normalization)	Peak Height
1	2.376	0.424	8.7
2	3.192	94.809	2664.0
3	4.162	4.767	46.7

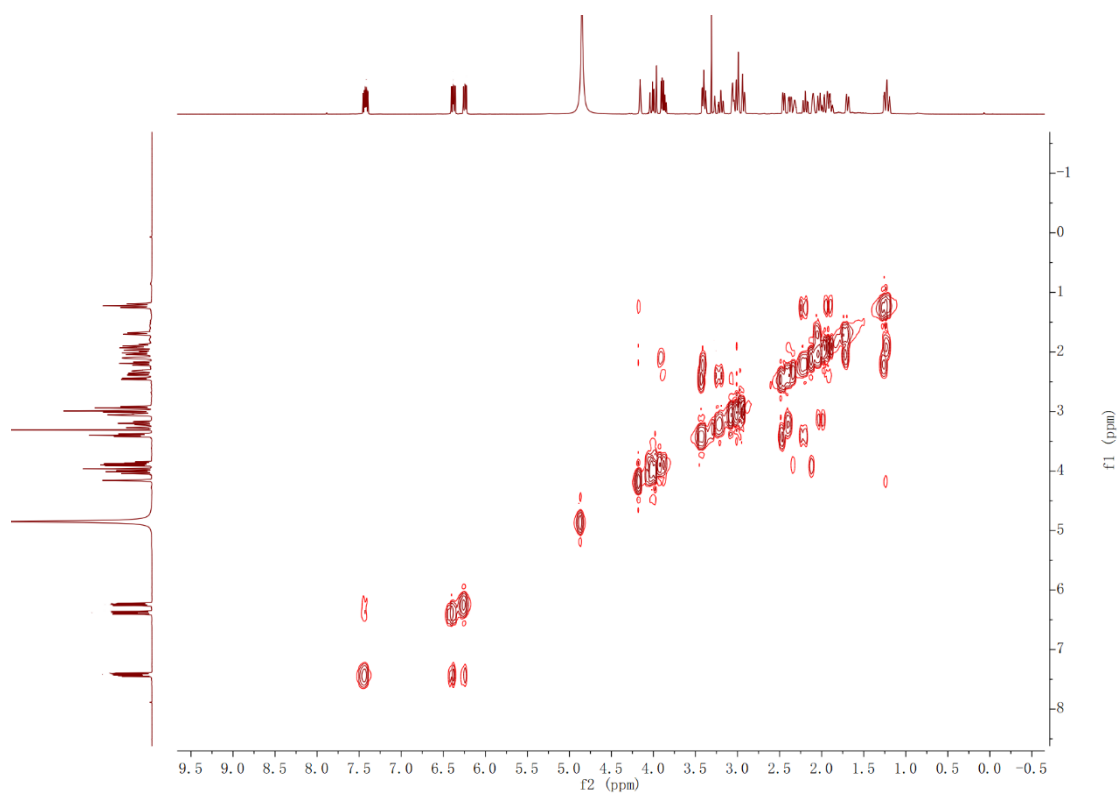
**Figure S1.** High Performance Liquid Chromatography (HPLC) of Sophobikushenine was performed using Agilent 1260 infinity II quaternary system with a UV detector and Poroshell 120 EC-C18 column (5  $\mu\text{m}$ , 4.6 mm  $\times$  150 mm; USA); Flow rate 1ml/min; Detector UV 220nm, Column temperature 35°C; Injection volume 10 $\mu\text{L}$ ; Elution program: 0-15min, MeOH-H<sub>2</sub>O, v/v: 5:95-95:5, 15min-20min, MeOH-H<sub>2</sub>O, v/v :95:5.



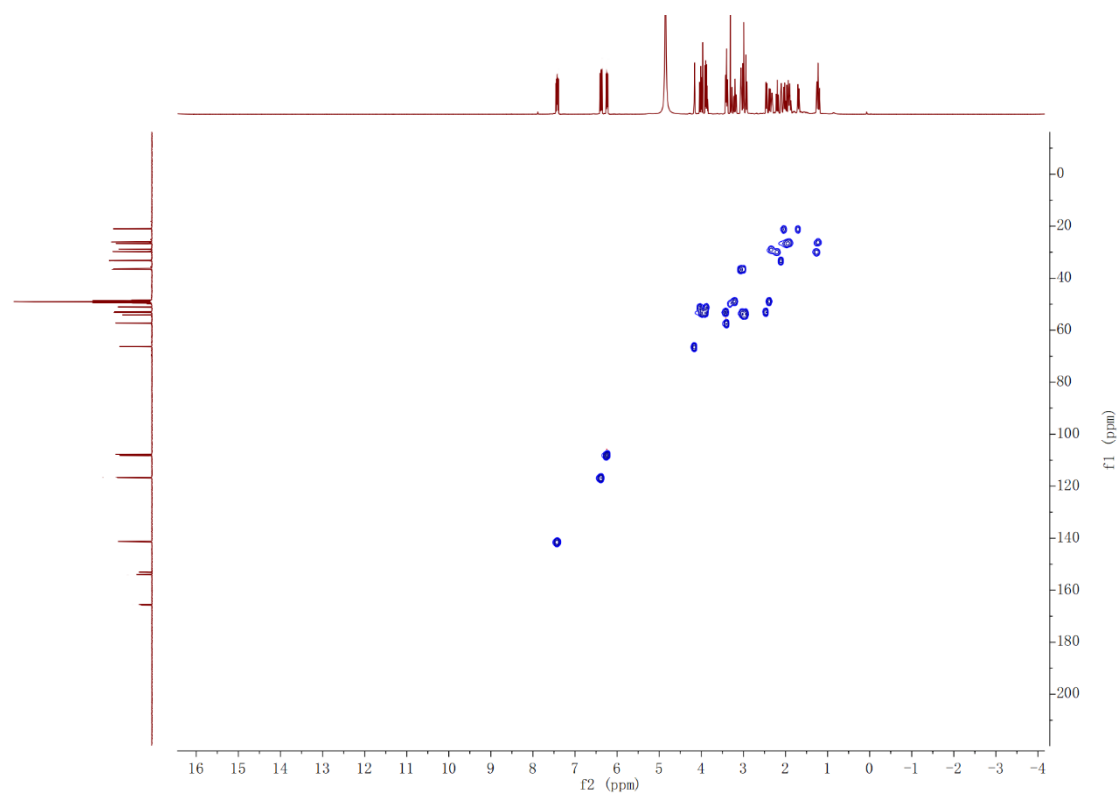
**Figure S2.** The <sup>1</sup>H NMR spectrum of Sophobikushenine in CD<sub>3</sub>OD (500 MHz)



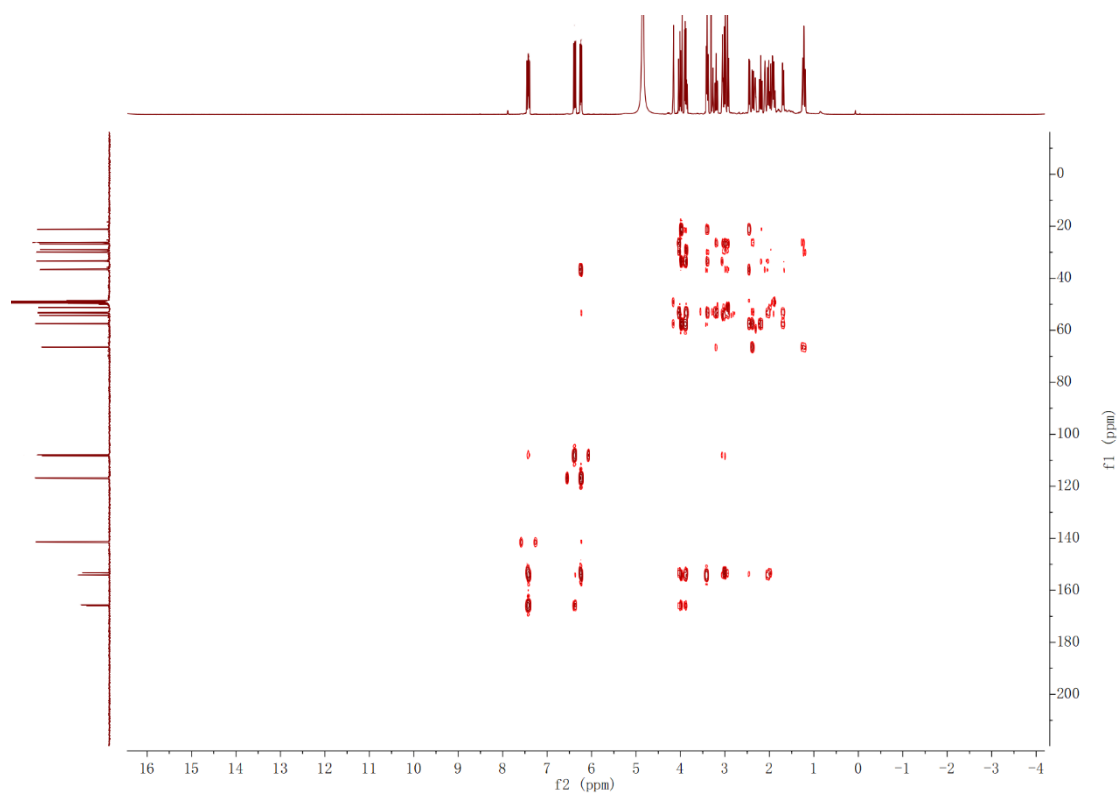
**Figure S3.** The  $^{13}\text{C}$  NMR spectrum of Sophobikushenine in  $\text{CD}_3\text{OD}$  (125 MHz)



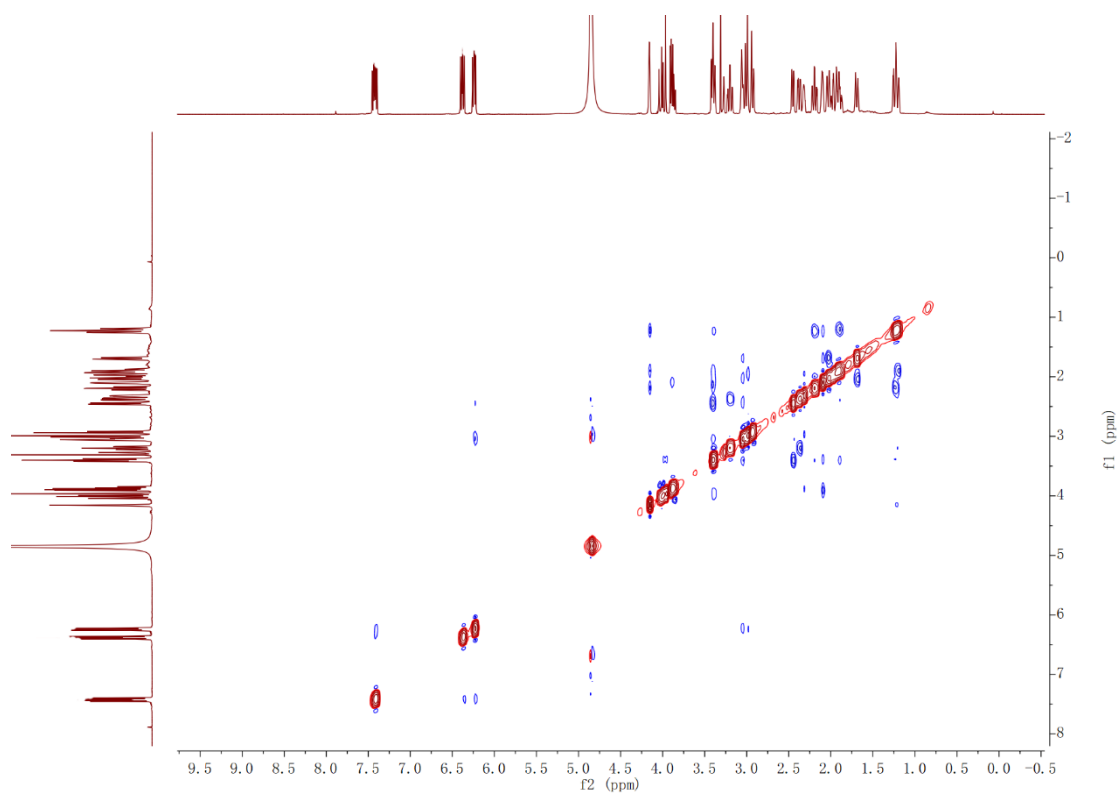
**Figure S4.** The  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of Sophobikushenine in  $\text{CD}_3\text{OD}$  (500 MHz)



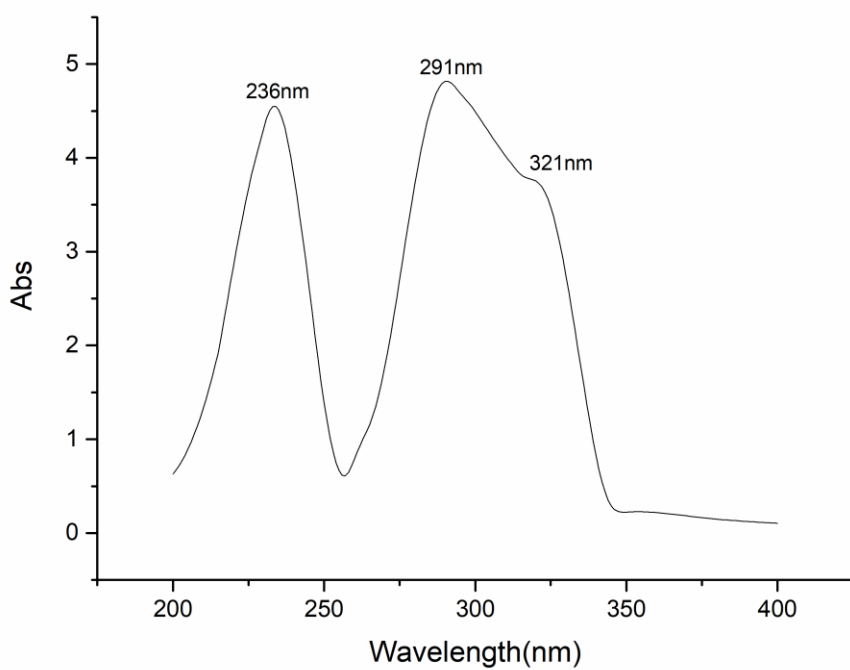
**Figure S5.** The HSQC spectrum of Sophobikushenine in CD<sub>3</sub>OD (500 MHz)



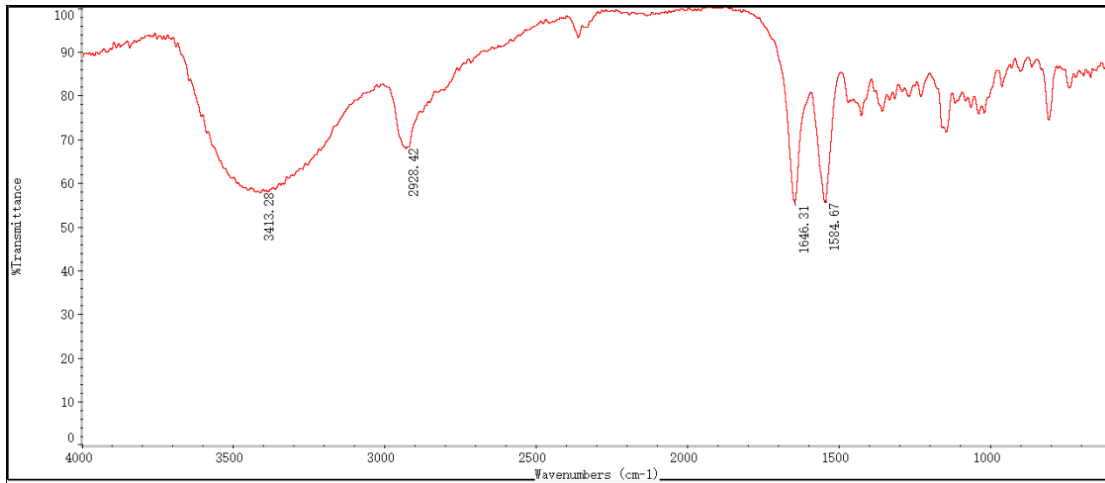
**Figure S6.** The HMBC spectrum of Sophobikushenine in CD<sub>3</sub>OD (500 MHz)



**Figure S7.** The NOESY spectrum of Sophobikushenine in CD<sub>3</sub>OD (500 MHz)

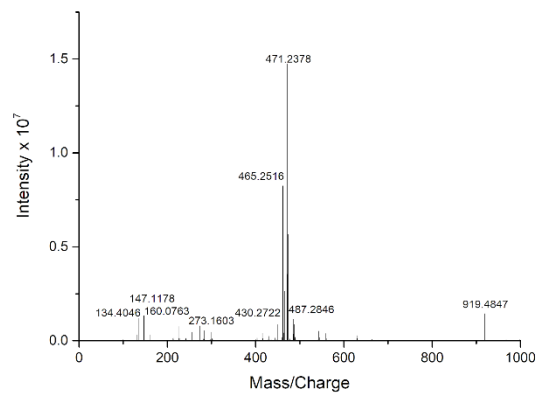


**Figure S8.** The UV spectrum of Sophobikushenine in MeOH

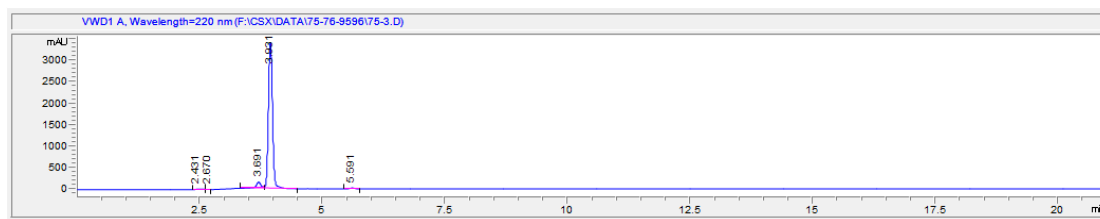


**Figure S9.** The IR spectrum (KBr) of Sophobikushenine

Mass Spectrum List Report					
<b>Analysis Info</b>			Acquisition Date 4/29/2021 8:45:22 PM		
Analysis Name	D:\Data\QL\0_A23_000001.d		Operator	solarix	
Method	4-13-DaDou		Instrument	solarix	
Sample Name					
Comment	PeptideMix NS=8 TF=1.2				
<b>Acquisition Parameter</b>					
Polarity	Positive	n/a	n/a	No. of Laser Shots	100
n/a	n/a	No. of Cell Fills	1	Laser Power	70.0 lp
Broadband Low Mass	53.8 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	1800.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a	Calibration Date	Fri Feb 21 02:36:54 2014
Pulse Program	basic	n/a	n/a	Data Acquisition Size	1048576
Source Accumulation	0.100 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.500 sec	n/a	n/a		
Flight Time to Acq. Cell	0.001 sec	n/a	n/a		

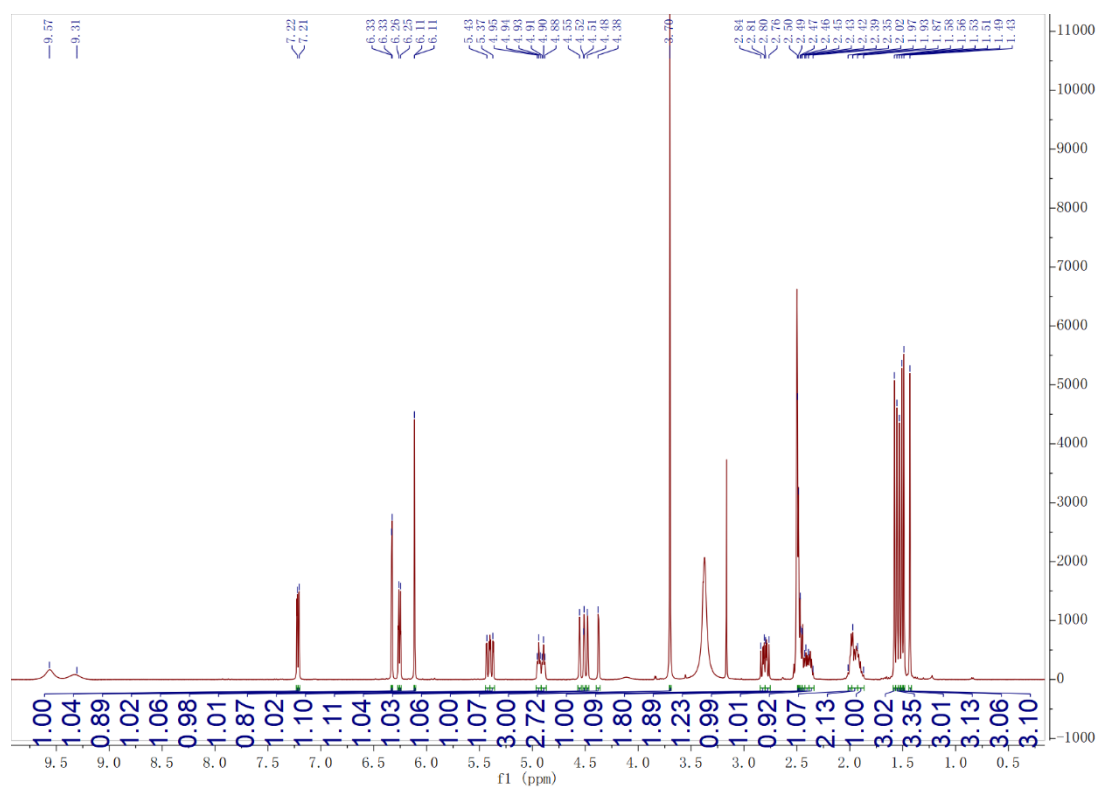


**Figure S10.** The HR-ESI-MS of Sophobikushenine

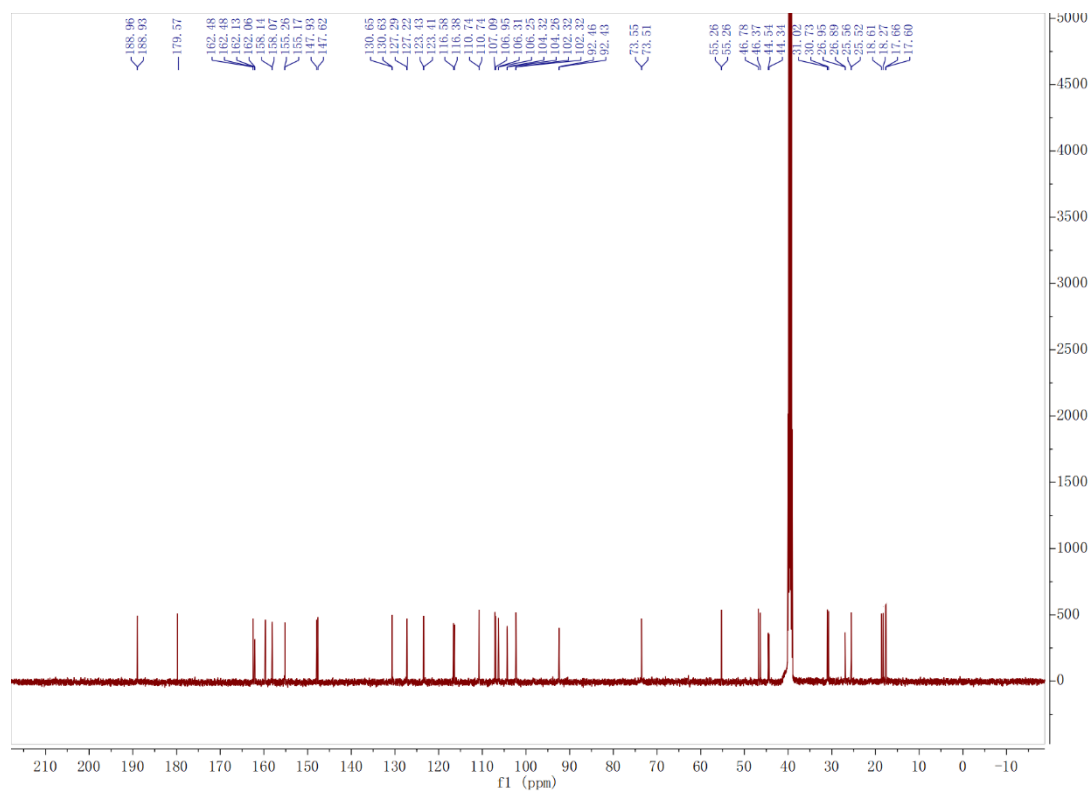


Number	Retention Time	Peak Area% (Area Normalization)	Peak Height
1	2.431	0.651	13
2	2.670	0.146	8.4
3	3.691	5.099	148.7
4	3.931	93.414	3374.6
5	5.591	0.691	23.9

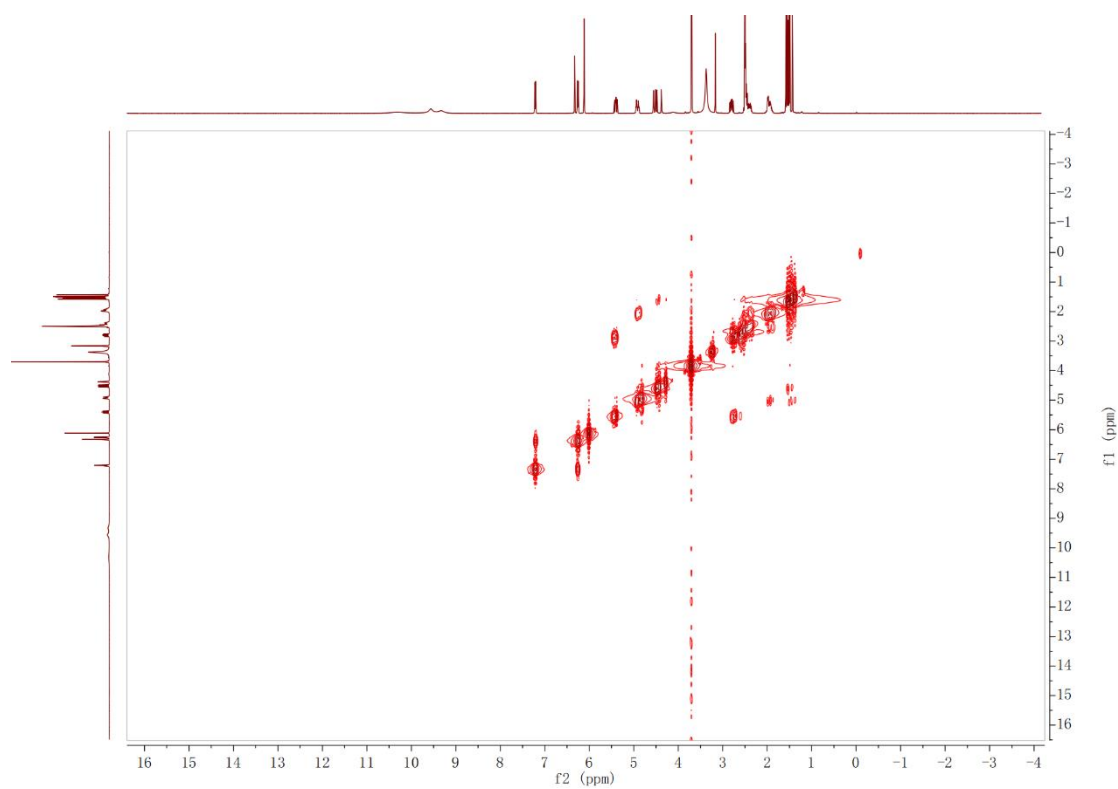
**Figure S11.** HPLC of Sophobiflavanone was performed using Agilent 1260 infinity II quaternary system with a UV detector and Poroshell 120 EC-C18 column (5  $\mu\text{m}$ , 4.6 mm  $\times$  150 mm; USA); Flow rate 1ml/min; Detector UV 220nm, Column temperature 35°C; Injection volume 10 $\mu\text{L}$ ; Elution program: 0-15min, MeOH-H<sub>2</sub>O, v/v: 5:95-95:5, 15min-20min, MeOH-H<sub>2</sub>O, v/v :95:5.



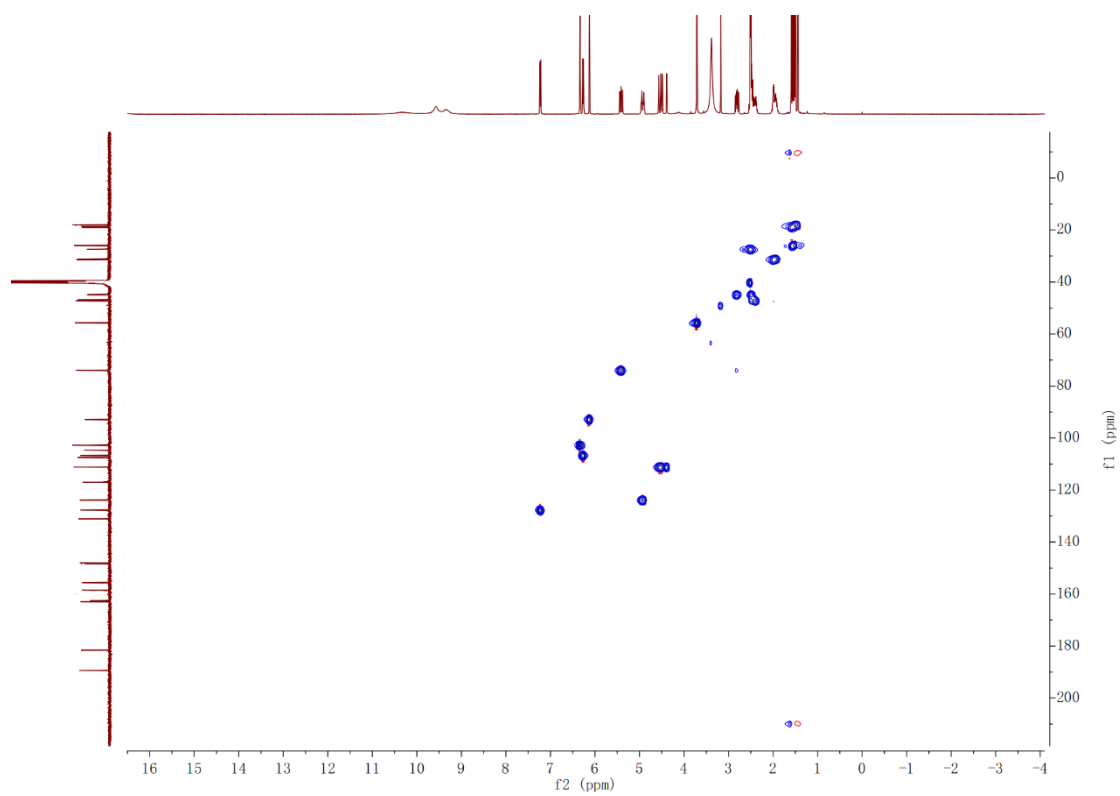
**Figure S12.** The <sup>1</sup>H NMR spectrum of Sophobiflavanone in DMSO (500 MHz)



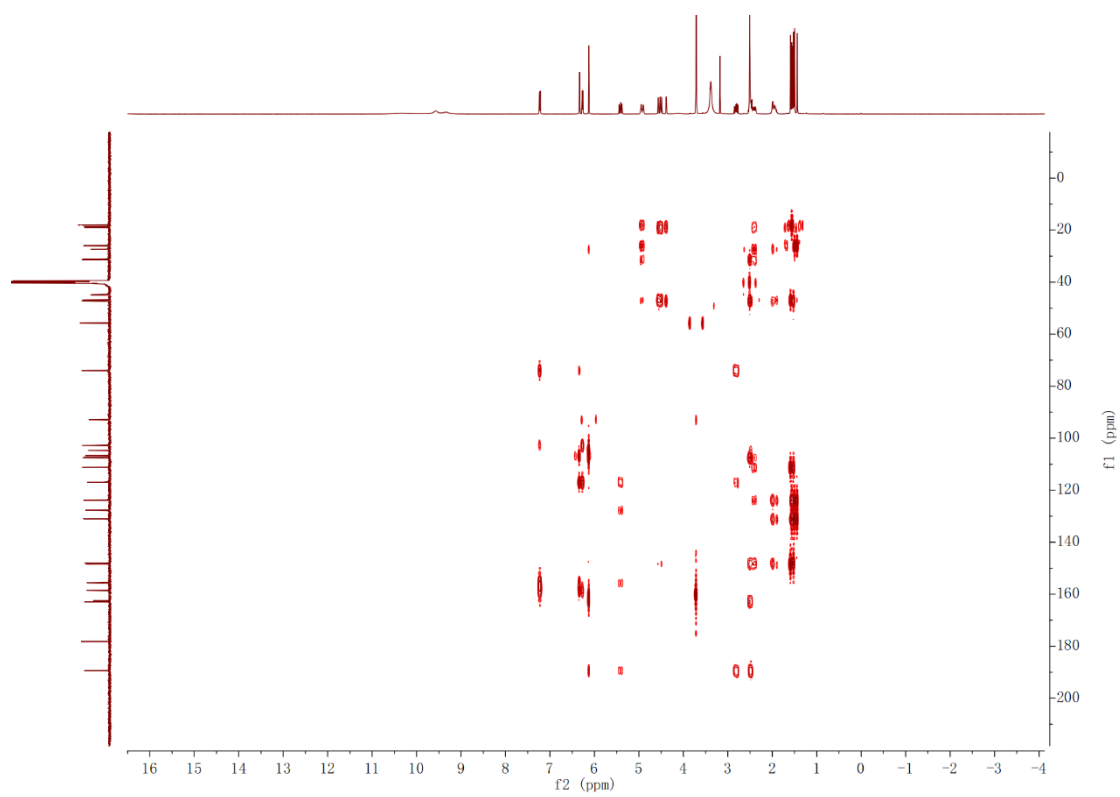
**Figure S13.** The  $^{13}\text{C}$  NMR spectrum of Sophobiflavanone in DMSO (125 MHz)



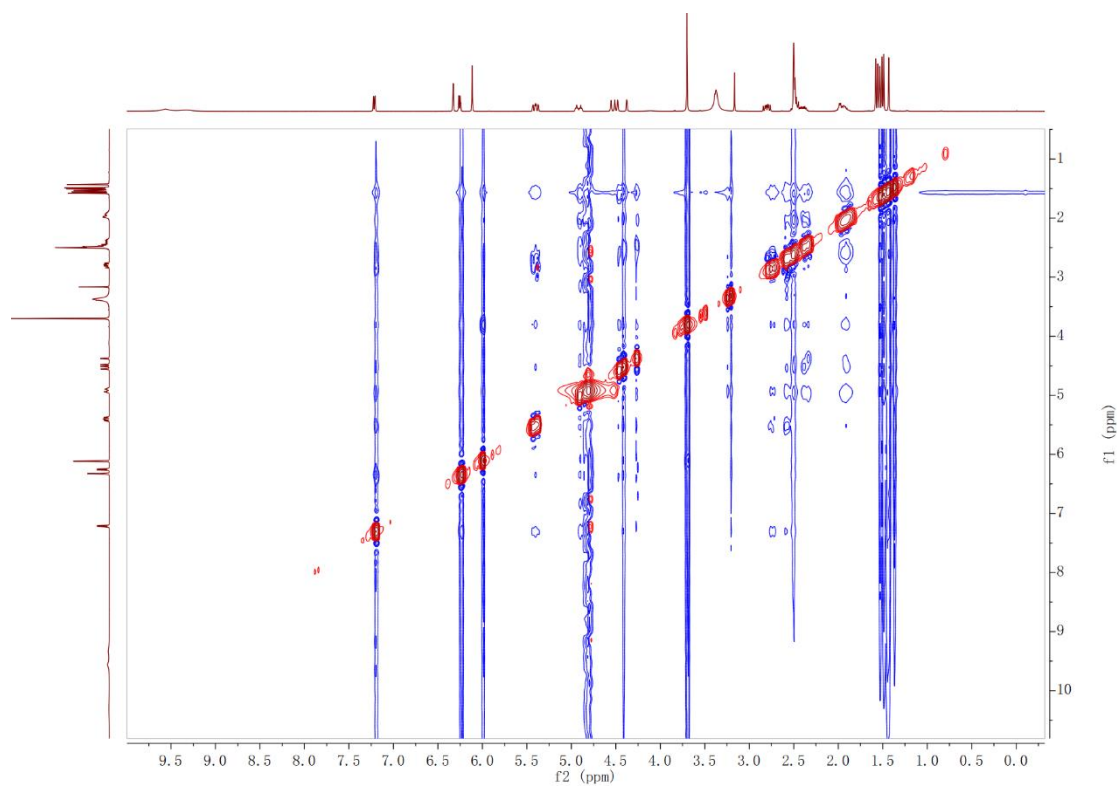
**Figure S14.** The  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of Sophobiflavanone in DMSO (500 MHz)



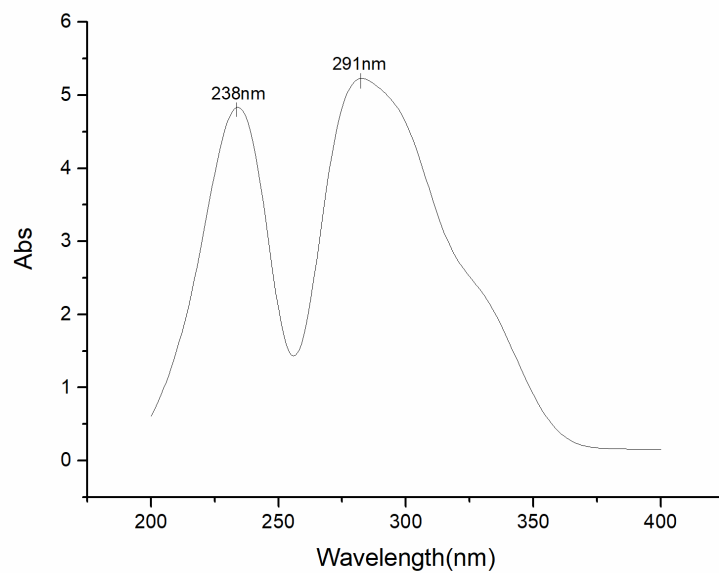
**Figure S15.** The HSQC spectrum of Sophobiflavanone in DMSO (500 MHz)



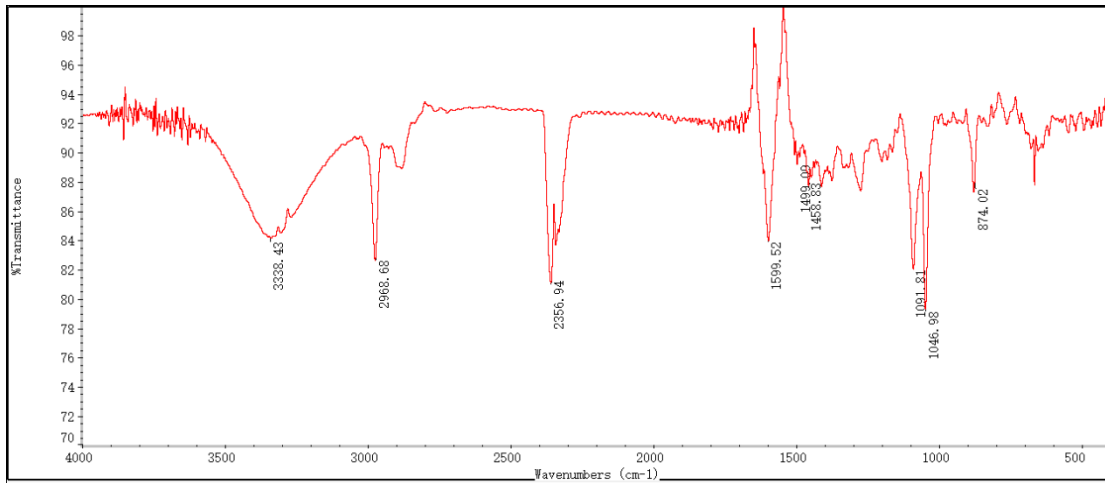
**Figure S16.** The HMBC spectrum of Sophobiflavanone in DMSO (500 MHz)



**Figure S17.** The NOESY spectrum of Sophobiflavanone in DMSO (500 MHz)

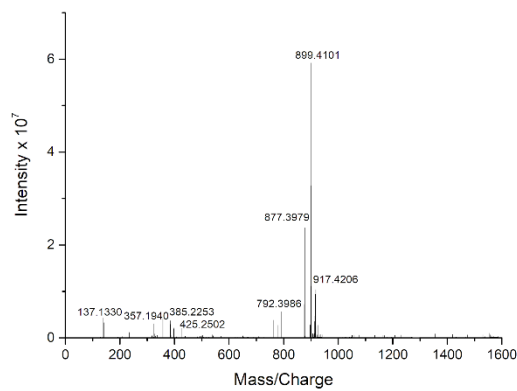


**Figure S18.** The UV spectrum of Sophobiflavanone in MeOH



**Figure S19.** The IR spectrum (KBr) of Sophobiflavanone

System Verification of Internal Mass Accuracy ESI Mode					
<b>Analysis Info</b>			Acquisition Date 7/23/2021 12:45:42 AM		
Analysis Name	D:\Data\1000_0_O17_000005.d		Operator	solarix	
Method	4-13-DaDou		Instrument	solarix	
Sample Name					
Comment	Glu-Fib 250amol				
<b>Acquisition Parameter</b>					
Polarity	Positive	n/a	n/a	No. of Laser Shots	100
n/a	n/a	No. of Cell Fills	1	Laser Power	70.0 lp
Broadband Low Mass	53.8 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	3000.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a	Calibration Date	Fri Feb 21 02:36:54 2014
Pulse Program	basic	n/a	n/a	Data Acquisition Size	1048576
Source Accumulation	0.100 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.500 sec	n/a	n/a		
Flight Time to Acq. Cell	0.001 sec	n/a	n/a		



**Figure S20.** The HR-ESI-MS of Sophobiflavanone